Cooper pairing and single particle properties of trapped Fermi gases

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We calculate the elementary excitations and pairing of a trapped atomic Fermi gas in the superfluid phase. The level spectra and pairing gaps undergo several transitions as the strength of the interactions between and the number of atoms are varied. For weak interactions, the Cooper pairs are formed between particles residing in the same harmonic oscillator shell. In this regime, the nature of the paired state is shown to depend critically on the position of the chemical potential relative to the harmonic oscillator shells and on the size of the mean field. For stronger interactions, we find a region where pairing occur between time-reversed harmonic oscillator states in different shells also.

I. INTRODUCTION

The trapping and cooling of trapped fermionic atomic gases is becoming a very active area of experimental research. Presently, temperatures as low as $\sim 0.2 T_F$ have been obtained for ^{40}K [1] and ^{6}Li [2–4] with T_F denoting the Fermi temperature. Part of the motivation for this impressive experimental progress is to observe the theoretically predicted transition to a superfluid state below a critical temperature T_c. With a large and attractive low energy effective interaction between two hyperfine states trapped, T_c for such a transition should be experimentally obtainable [5].

The purpose of the present paper is examine the elementary excitations of the ground state for an atomic superfluid gas in a spherical harmonic trap. Varying the interaction strength and the number of particles in the trap a number of interesting transitions in the level spectra and pairing gaps occur. We calculate these transitions by solving the Bogoliubov-deGennes equations both numerically and analytically using a degenerate shell pairing approximation for weak interactions and semiclassical methods for many particles. An understanding of such elementary excitations is important if one wants to predict the response of the gas to various single particle probes. Moreover, these elementary excitations are also the building blocks, if one wants to calculate collective properties of the superfluid gas.

The paper is organized as follows: In sec. II, we set up the basic formalism used in the rest of the paper. We then in sec. III discuss the weak pairing regime, where Cooper pairs are formed only between particles within the same harmonic oscillator shell. The qualitatively different limit of strong pairing is discussed in sec. IV, where Cooper pairs are formed between particles residing in different shells. We finally summarize our results in sec. V.

II. BASIC EQUATIONS

We consider a dilute gas of N fermionic atoms of mass m in two hyperfine states $|\sigma =\uparrow, \downarrow\rangle$ trapped by a spherically symmetric harmonic oscillator (h.o.) potential at zero temperature. The numbers N_σ of atoms trapped in each hyperfine state are assumed to be equal such that $N = 2N_\sigma$ as this is the optimum situation for Cooper pairing. We assume that the atoms interact through an attractive s-wave scattering length, $a < 0$. The Hamiltonian is then given by

$$H = \sum_{i=1}^{N} \left(\frac{\mathbf{p}_i^2}{2m} + \frac{1}{2}m\omega^2 r_i^2 \right) + 4\pi \frac{\hbar^2 a}{m} \sum_{i<j} \delta(\mathbf{r}_i - \mathbf{r}_j). \quad (1)$$

It should be noted that to reproduce the correct 2-body scattering properties one needs to use a pseudo-potential $\delta(\mathbf{r})\partial_r r$ instead of a simple delta-function for the interaction term in Eq.(1). This is important when the pairing correlations are to be calculated [6]. We will return to this point in sec. III. In a non-interacting system the Fermi energy is

$$E_F = (n_F + 3/2)\hbar\omega \simeq (3N)^{1/3}\hbar\omega, \quad (2)$$

where n_F is the h.o. quantum number at the Fermi surface. For a large number of particles $n_F = (3N)^{1/3}$.

Interactions result in a mean field potential which is for a large number of particles given by the Thomas-Fermi approximation (TF)

$$U(r) = 2\pi \frac{\hbar^2 a}{m}\rho(r), \quad (3)$$

where the particle density is

$$\rho(r) = k_F^3(r)/3\pi^2 \simeq \rho_0 \left(1 - r^2/R_{TF}^2 - U(r)/E_F \right)^{3/2} \quad (4)$$

inside the cloud $r \leq R_{TF} = a_{osc}\sqrt{2n_F + 3}$, where $a_{osc} = \sqrt{\hbar/m\omega}$ is the oscillator length, and $\rho_0 = (2n_F)^{3/2}/3\pi^2 a_{osc}^3$ is the central density [7]. $k_F(r)$ is the TF Fermi wave-number and the Fermi energy is

$$E_F = \hbar^2 k_F^2(r)/2m + (1/2)m\omega^2 r^2 + U(r). \quad (5)$$

In dilute systems the interactions contribute a mean field weak compared to the confining potential, i.e., $U(r)$ can be neglected in Eq. (4).

The system is *dilute* when the Fermi energy is large compared to the mean field energy, $E_F \gg U$, or equivalently $k_F|a| \simeq \rho^{1/3}|a| \simeq n_F^{1/2}|a|/a_{osc} \ll 1$. *Dense* Fermi

systems, $k_F|a|\gtrsim 1$, are studied in Refs. [8]. In *very dilute* systems also the h.o. energy exceeds the mean field potentials, $\hbar\omega \gg U$, or equivalently $n_F^{3/2}|a|/a_{osc} \ll 1$.

The h.o. levels are highly degenerate with states having angular momenta $l = n, n-2\ldots, 0$ (n even) or $l = n, n-2\ldots, 1$ (n odd) due to the $U(3)$ symmetry of the 3D spherically symmetric h.o. potential. However, interactions split this degeneracy. The splitting can be calculated perturbatively in the very dilute limit. From the radial h.o. wave-function $\mathcal{R}_{n_Fl}(r)$ for the state with angular momentum l and $(n_F - l)/2$ radial nodes in the h.o. shell n_F, the single particle energies with respect to the Fermi energy are within the WKB approximation [9]

$$\xi_{n_F,l} = \int U(r)|\mathcal{R}_{nl}(r)|^2 r^2 dr$$
$$= \frac{4\sqrt{2}}{3\pi}\frac{a}{a_{osc}}n_F^{3/2}\hbar\omega\left[\frac{4}{3\pi} - \frac{l(l+1)}{4\pi n_F^2}\right]. \quad (6)$$

The mean field energies are proportional to the coupling and $n_F^{3/2}$ and are split like rotational bands with a prefactor that is smaller than the average mean field energy by a factor $\sim 3/16$. The relative small splitting reflects the fact that the mean field potential is almost quadratic in r and the anharmonic terms therefore small.

We plot in figure 1 the different regions of pairing for the trapped gas as a function of the number of particles and the coupling strength.
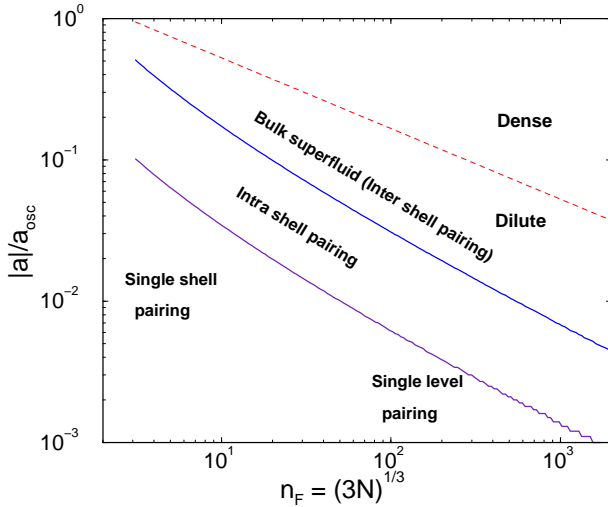

FIG. 1. The different level structures and pairing gaps in traps are displayed vs. the two dimensionless parameters: The energy quantum number n_F of the highest shell occupied and the interaction strength $|a|/a_{osc}$. The dotted line separates the dense and dilute trapped gases. Above the blue full line $\Delta = \hbar\omega$, the system has coherence length smaller than the system size and pairing occurs between particles in different harmonic oscillator shells. Below, a region exists where there is only pairing between particles in the same shell but many h.o. shells contribute to the total pairing field. Below the purple line $G\ln(n_F) \simeq 0.1\hbar\omega$, there is only pairing in the shell at the chemical potential leading to the gap $\Delta \simeq G$ for small systems whereas pairing takes place in a single l-level only for large systems. It should be noted that the transitions between the different regions are smooth.

We shall below calculate pairing energies by solving the Bogoliubov-de Gennes (BdG) equations numerically and also analytically in certain limits exploiting known properties of the known h.o. wave-functions and single particle levels. The BdG equations read [10]:

$$E_\eta u_\eta(\mathbf{r}) = [\mathcal{H}_0 + U(\mathbf{r})]u_\eta(\mathbf{r}) + \Delta(\mathbf{r})v_\eta(\mathbf{r})$$
$$E_\eta v_\eta(\mathbf{r}) = -[\mathcal{H}_0 + U(\mathbf{r})]v_\eta(\mathbf{r}) + \Delta(\mathbf{r})u_\eta(\mathbf{r}). \quad (7)$$

Here, $\mathcal{H}_0 = -(\hbar^2/2m)\nabla^2 + U_0(\mathbf{r}) - \mu_F$, $U(\mathbf{r}) \equiv g\langle\hat{\psi}_\sigma^\dagger(\mathbf{r})\hat{\psi}_\sigma(\mathbf{r})\rangle = g\rho_\sigma(\mathbf{r})$ is the Hartree potential, and $\hat{\psi}_\sigma(\mathbf{r})$ is the field operator that annihilates an atom in spin state σ at position $\mathbf{r}$. The coupling constant is $g = 4\pi a\hbar^2/m$ with $a < 0$ for an attractive interaction leading to pairing, and μ_F denotes the chemical potential. The pairing field is defined as $\Delta(\mathbf{R}) \equiv -g\lim_{r\to 0}\partial_r[r\langle\hat{\psi}_\uparrow(\mathbf{R} + \mathbf{r}/2)\hat{\psi}_\downarrow(\mathbf{R} - \mathbf{r}/2)\rangle]$ and can be taken to be real [6]. The quasi particles with energies E_η are described by the Bogoliubov wave functions $u_\eta(\mathbf{r})$ and $v_\eta(\mathbf{r})$.

For spherical symmetry, the Bogoliubov wave functions from Eq.(7) have definite angular momentum quantum numbers lm and can be written in the form $u_{\eta lm}(\mathbf{r}) = r^{-1}u_{\eta l}(r)Y_{lm}(\theta,\phi)$ and $v_{\eta lm}(\mathbf{r}) = r^{-1}v_{\eta l}(r)Y_{lm}(\theta,\phi)$ with an energy energy $E_{\eta l}$. To obtain analytical results for the pairing energy in some limits, it is convenient to expand the Bogoliubov wavefunctions in the complete set of unperturbed spherical Harmonic oscillator functions by writing $u_{\eta lm}(\mathbf{r}) = \sum_n u_{\eta nl}\phi_{nlm}^0(\mathbf{r})$ and $v_{\eta lm}(\mathbf{r}) = \sum_n v_{\eta nl}\phi_{nlm}^0(\mathbf{r})$ with $\phi_{nlm}(\mathbf{r}) = \mathcal{R}_{nl}(r)Y_{lm}(\theta,\phi)$. We have $\mathcal{H}_0\phi_{nlm}^0(\mathbf{r}) = \xi_n\phi_{nlm}^0(\mathbf{r})$ with $\xi_n = (n+3/2)\hbar\omega - \mu_F$ [$l = n, n-2\ldots, 0$ (n even) or $l = n, n-2\ldots, 1$ (n odd)]. Using this expansion, the BdG equations become for a given lm:

$$E_{\eta l}u_{\eta nl} = \sum_{n'}[\langle nl|\mathcal{H}|n'l\rangle u_{\eta n'l} + \langle nl|\Delta(r)|n'l\rangle v_{\eta n'l}]$$

$$E_{\eta l}v_{\eta nl} = \sum_{n'}[\langle nl|\Delta(r)|n'l\rangle u_{\eta n'l} - \langle nl|\mathcal{H}|n'l\rangle v_{\eta n'l}]. \quad (8)$$

Here $\mathcal{H} = \mathcal{H}_0 + U(\mathbf{r})$ and the matrix elements are defined as $\langle nl|\hat{A}|n'l\rangle \equiv \int_0^\infty \mathcal{R}_{nl}(r)\hat{A}\mathcal{R}_{n'l}(r)r^2 dr$.

2

We will examine certain regimes for which one can derive approximate analytical results from Eq.(8) [or Eq.(7)] and thus for the Cooper pairing in a harmonic trap. We keep the temperature $T = 0$ for the remaining part of this paper in order to examine the ground state properties of the gas. The nature of the paired state depends on the relative magnitude of the Hartree field $U(r)$, the trap level spacing $\hbar\omega$, and the pairing field $\Delta(r)$.

III. INTRA SHELL PAIRING

In this section, we examine the case when the interaction is so weak, that it only induces pairing between particles within the same harmonic oscillator shell [$n = n'$ in Eq.(8)], hence the term *intra* shell pairing. In this regime the pairing energy is smaller than the trap level spacing $2\hbar\omega$ between states with the same angular momentum quantum number l [The Cooper pairing is between states with the angular quantum numbers (l, m) and $(l, -m)$]. We ignore for the time being the splitting of the harmonic oscillator shells due to the Hartree field. The harmonic oscillator shells therefore have the energies $\tilde{\xi}_{nl} \simeq \xi_n = (n + 3/2)\hbar\omega - \mu_F$ with the angular momentum quantum number $l = n, n - 2\ldots, 0$ (n even) or $l = n, n - 2\ldots, 1$ (n odd). The strength of the pairing between states with quantum numbers (n, l) and (n', l) in Eq.(8) is given by the matrix element

$$\langle nl | \Delta(r) | n'l \rangle = \int_0^\infty dr r^2 \Delta(r) \mathcal{R}_{nl}(r) \mathcal{R}_{n'l}(r). \quad (9)$$

The radial functions $\mathcal{R}_{nl}(r)$ in general change sign as a function of r. In the ground state however, $\Delta(r)$ has a definite sign (chosen to be positive in the present case) as any oscillations in the pairing field in general costs energy. We therefore see that the "inter-shell" matrix elements with $n \neq n'$ will be suppressed due to the oscillating phase of $\mathcal{R}_{nl}(r) \mathcal{R}_{n'l}(r)$ as compared to the "intra-shell" matrix elements with $n = n'$. The weak pairing regime considered in this section is characterized by the fact that the inter-shell matrix elements can be ignored. A simple perturbative calculation reveals that the parameter determining the importance of the inter-shell matrix elements is $|\langle nl | \Delta(r) | n'l \rangle| / \hbar\omega$. When this parameter is small these matrix elements can be ignored and we are in the intra-shell pairing regime. For stronger coupling, this parameter is no longer small and the inter-shell matrix elements changes the solution to the self-consistent and thus non-linear gap equations qualitatively. We will describe this in detail in sec. IV.

Ignoring all inter-shell matrix elements, Eq.(8) splits into simple 2×2 matrix equations for each pair of quantum numbers (n, l). For a given set of quantum numbers (n, l), we obtain the usual solution $u_{nl} = (1 + \xi_n / E_{nl})/2$, $v_{nl} = (1 - \xi_n / E_{nl})/2$ with $E_{nl} = (\xi_n^2 + \Delta_{nl}^2)^{1/2}$ and $\Delta_{nl} = \langle nl | \Delta(r) | nl \rangle$. Ignoring for the moment the regularization of the gap function, the self-consistent equation

for the pairing field becomes:

$$\Delta(r) = \frac{|g|}{2} \sum_{n,l} \frac{2l + 1}{4\pi} \frac{\Delta_{nl}}{E_{nl}} \mathcal{R}_{nl}^2(r) \quad (10)$$

where the factor $2l + 1$ comes from the summation over the angular quantum number m. The nature of the self-consistent solution of the BdG equations depends on the position of the chemical potential μ_F relative to the trap levels. We will now examine two opposite cases of interest.

A. Partly filled Shell

When the chemical potential is at a harmonic oscillator shell, i.e. $\mu_F = (n_F + 3/2)\hbar\omega$, this shell is partly filled for $T = 0$. This is the typical situation physically, whereas the case of a completely filled shell corresponding to $\mu_F = (n_F + 2)\hbar\omega$ at $T = 0$ occur only for "magic" numbers of trapped particles. In this section we will provide a analytical solution to the pairing problem when the interaction is so weak that only intra shell pairing is significant and $\mu_F = (n_F + 3/2)\hbar\omega$. We will show that for very weak interaction the main contribution to the pairing correlations originate from the partly filled shell at the chemical potential ($n = n_F$), whereas for stronger interactions the contribution to the pairing from shells away from the chemical potential ($n \neq n_F$) is dominant. Using Eq.(9) and Eq.(10), the self-consistent equation for the intra shell pairing matrix elements reads

$$\Delta_{nl} = \frac{|g|}{2} \sum_{l'} \frac{2l' + 1}{4\pi} \int_0^\infty dr r^2 \mathcal{R}_{nl}^2(r) \mathcal{R}_{n_F l'}^2(r) +$$

$$\frac{|g|}{2} \sum_{n' \neq n_F, l'} \frac{2l' + 1}{4\pi} \frac{\Delta_{n'l'}}{\sqrt{\xi_{n'}^2 + \Delta_{n'l'}^2}} \int_0^\infty dr r^2 \mathcal{R}_{nl}^2(r) \mathcal{R}_{n'l'}^2(r) \quad (11)$$

where the first term singles out the contribution from the shell at the chemical potential. Notice that for this shell, $\xi_{n_F} = 0$ such that $E_{n_F} = \Delta_{n_F l}$. Equation (11) gives the strength of the pairing as a function of the angular momentum l of the particles forming the Cooper pair and their shell quantum number n. The l-dependence of the pairing, determined through the integral $\int dr r^2 \Delta(r) \mathcal{R}_{nl}^2(r)$, is rather weak; we will later show that $|\Delta_{n,l=n} - \Delta_{n,l=0}| / \Delta_{n,l=0} \ll 1$. It is therefore not important for the present analysis and we define the l-averaged pairing strength as $\Delta_n = \sum_l (2l + 1)\Delta_{nl} / \Omega_n$ with $\Omega_n = \sum_l (2l + 1) = (n + 1)(n + 2)/2$ being the (single spin) degeneracy of the harmonic oscillator shell with energy $(n + 3/2)\hbar\omega$. For $n \gg 1$, we can use the Thomas-Fermi identity

$$\sum_l \frac{(2l + 1)}{4\pi} \mathcal{R}_{n'l}^2(r) = \frac{\partial \rho_\sigma(r)}{\partial n'} = \frac{\sqrt{2n' + 3}}{2\pi^2 a_{osc}^3} \sqrt{1 - r^2 / R_{TF}^2(n')} \quad (12)$$

with $R_{TF}(n') = \sqrt{n' + 3/2} a_{osc}$. Here, ρ_σ is the density from a single hyperfine state when shells up to energy

$(n'+3/2)\hbar\omega$ are occupied; $\partial\rho_\sigma(r)/\partial n'$ therefore should be understood as the derivative of the density with respect to the highest harmonic oscillator shell occupied. The pairing strength Δ_n depends weakly on n for the shells around $n = n_F$ which mainly contribute to the pairing and we therefore approximate $\Delta_n \simeq \Delta_{n_F} \equiv \Delta$. Equation (11) then becomes

$$\Delta = G + \nu G \sum_{\substack{n \neq n_F}}^{n<2n_F} \frac{\Delta}{\sqrt{[(n-n_F)\hbar\omega]^2 + \Delta^2}}, \quad (13)$$

where we have defined

$$G = \frac{|g|}{2} \frac{\int dr\, r^2 [\partial_n \rho_\sigma(r)|_{n_F}]^2}{\int dr\, r^2 \partial_n \rho_\sigma(r)|_{n_F}} = \frac{32\sqrt{2n_F+3}}{15\pi^2} \frac{|a|}{a_{osc}} \hbar\omega. \quad (14)$$

The correction factor ν arises because the overlap integrals in the second term in Eq.(11) depend on the shell number n'. We approximate this dependence by averaging the factor $\sqrt{n'}$, which gives $\nu = \int_0^{2n_F} n^{1/2} dn / 2n_F^{3/2} = 2^{3/2}/3$. We have introduced the cut-off $n < 2n_F$ in the sums which models as a first approximation the more rigorous regularization procedure described in Ref. [6] that is required for a delta-function pseudo-potential. Such a procedure can for the present purpose be approximated by a cut-off of $n < 2n_F$ essentially due to the fact that the Lippman-Schwinger eqn. for two particle scattering appearing in the regularization procedure contains a single particle Green's function which is odd around the Fermi surface whereas the contribution to the pairing is even due to the particle-hole symmetry.

When $\Delta \ll \hbar\omega$ we can expand and find the gap

$$\Delta = \frac{G}{1 - 2\nu \ln(e^\gamma n_F)\frac{G}{\hbar\omega}}. \quad (15)$$

Here, $\gamma \simeq 0.577$ is Eulers constant. For very weak interactions, $G\ln(n_F) \ll \hbar\omega$, the gap is simply $\Delta = G$. This corresponds to the limit where pairing only occurs in the shell right at the chemical potential ($n = n_F$). The result $\Delta = G$ was also obtained in ref. [9] using a different approach (the seniority scheme). As $G\ln(n_F)$ increases the gap increases and $\Delta > G$ due to intra shell pairing in shells away from the chemical potential. For $G\ln(n_F) \sim 1/2$, Eq. (15) diverges. However, at the same time the shell pairing ansatz leading to Eq. (11) breaks down as will be described in detail in the following section.
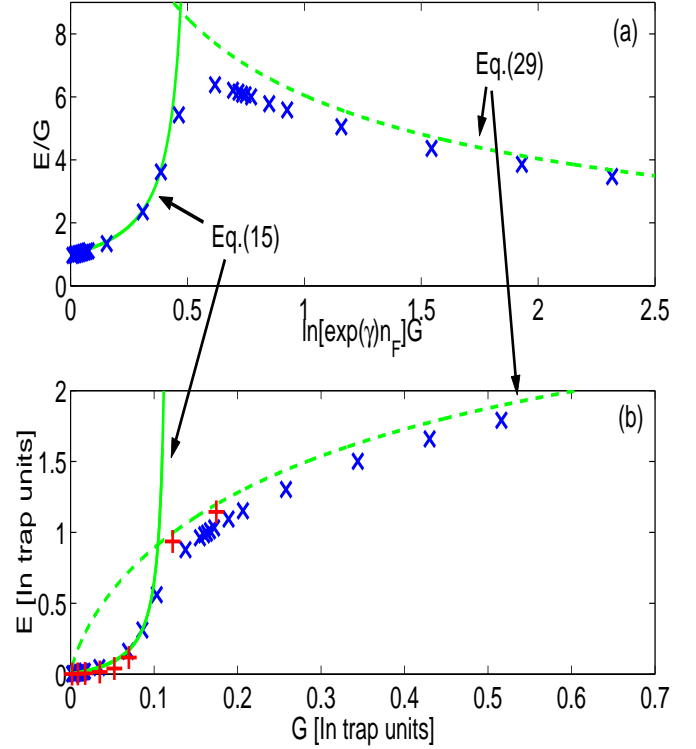

FIG. 2. The lowest quasi particle energy $E_{l=0}$ divided by the effective coupling strength G as a function of $G\ln[\exp(\gamma)n_F]$ (in units of $\hbar\omega$) (a). Figure (b) depicts $E/\hbar\omega$ as a function of $G/\hbar\omega$. $\mu_F = 51.5\hbar\omega$. Plusses and crosses are with and without the Hartree field respectively.

In fig. (2a), we plot the lowest l averaged quasi particle energy $E = \Delta$ (since $\xi_{n_F} = 0$) divided by the effective coupling strength G as a function of $G\ln[\exp(\gamma)n_F]$. The solid curve is calculated from Eq.(15) whereas the $\times$'s are results obtained from numerical calculations as described in ref. [6]. We have chosen $n_F = 50$ for the numerical calculations corresponding to $\sim 2 \times 10^4$ particles trapped in each of the two hyperfine states. Note that according to Eq.(15), E/G in terms of $G\ln[\exp(\gamma)n_F]$ is a *universal* function independent of the size of the system (i.e. independent of n_F) as long as the system is in the intra shell pairing regime. In this regime, we see that there is excellent agreement between Eq.(15) and the numerical results. For stronger coupling, the intra shell pairing assumption breaks down and the numerical results differ qualitatively from Eq.(15). The nature of the Cooper pairs undergoes a transition to a region where the pairing between particles in different harmonic shells is significant. The transition in the nature of the pairing is clearly visible in fig. (2a) since E/G changes from being an increasing to a decreasing function of $G\ln[\exp(\gamma)n_F]$ when the intershell pairing becomes dominant. We will examine the intershell pairing in detail in section IV. Of course, the pairing strength is a monotonic increasing function of the coupling strength G as shown in fig. (2b).

4

For weak pairing, $[G\ln(n_F) \ll \hbar\omega]$ we find $\Delta = G$ in agreement with the analysis above. In this regime there is only significant pairing in the shell at the chemical potential. For stronger interaction with $G\ln(n_F) \gtrsim 0.1\hbar\omega$, the Cooper pairing is still only between particles within the same shell, but shells away from the chemical potential $(n \neq n_F)$ contribute significantly to the pairing energy as predicted by Eq.(15).

The reason that shells away from the chemical potential contribute to the pairing for stronger coupling is that it becomes energetically favorable to partially occupy these shells in order to make a coherent state with stronger spatial overlap between the particles forming the Cooper pairs.

We will now briefly examine the dependence of the pairing strength $\Delta_{n_F l}$ given by Eq.(11) on the angular momentum quantum number l. It is assumed that we are in the very weak coupling regime $[\ln(n_F)G \ll 1]$ such that such that only the shell at the chemical potential $n = n_F$ contributes to the pairing. Using Eq.(12), $\mathcal{R}_{n_F l = n_F}(r) \propto r^{n_F}\exp(-r^2/2a_{osc}^2)$, and the semiclassical approximation $r\mathcal{R}_{n_F l=0}(r) \simeq [k(r)]^{-1/2}\sin(\int^r dr'k(r') + \phi)$ with $k(r) = \sqrt{2n_F - r^2/a_{osc}^2}$, the radial integral in Eq.(11) can easily be solved for $l = 0$ (n_F even) and $l = n_F$ yielding

$$\frac{E_{n_F l}}{G} = \frac{\Delta_{n_F l}}{G} = \begin{cases} 15/16 & , \ l = 0 \\ 15\pi/(32\sqrt{2}) & , \ l = n_F \end{cases} \quad (16)$$

with G given by Eq.(14). From Eq.(16), we see that $|\Delta_{n_F, l=n_F} - \Delta_{n_F, l=0}|/\Delta \simeq 0.10 \ll 1$ thereby justifying the l averaging of the pairing strength described above.
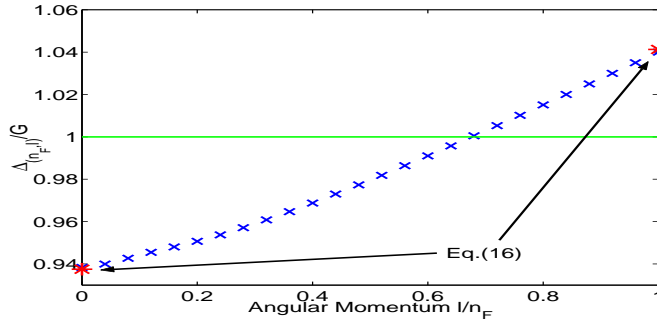

FIG. 3. The lowest quasi particle energies $E_{n_F l} = \Delta_{n_F l}$ (in units of G) as a function of the angular momentum l/n_F for $\mu_F = 51.5\hbar\omega$ and $G = 1.75 \times 10^{-4}\hbar\omega$.

Figure (3) shows the l-dependence of the lowest quasi particle excitation energy $E_{n_F l} = \Delta_{n_F l}$ for the same parameters as for fig. (2) and $G/\hbar\omega = 1.75 \times 10^{-4} \ll \ln(n_F)^{-1}$. The ×'s indicate the numerical results, the ∗'s indicate the results given by Eq.(16). We also plot the l averaged value $\Delta = G$ as a solid line. The numerical results agree very well with the analytical predictions of Eq. (16) up to $1/n_F$ corrections. We notice that the l-dependence is weak thereby justifying the l-averaging of the pairing assumed above. Again, one should note

that fig. (3) is universal in the sense that it is independent of the size of the system given by n_F; one always has $0 \le l/n_F \le 1$ and $E_{n_F l}/G$ is independent of n_F for $\ln(n_F)G \ll 1$ as can be seen from Eq.(16).

B. Filled Shell

We now examine the case when the chemical potential is exactly between two harmonic oscillator shells, i.e. $\mu_F = (n_F + 2)\hbar\omega$. This case corresponds to shells up to and including $n = n_F$ being completely filled and shells with $n > n_F$ empty when there is no pairing. As we will see, this situation differs qualitatively from the case considered in sec. (III A) in the sense that the pairing is zero below a certain critical coupling strength G_c. Again, we are in this section in the weak pairing regime such that only intra shell pairing is significant. Thus, Eq.(10) is still valid and leads to a gap equation analogous to Eq.(11), however, excluding the first term corresponding to pairing in the shell at the chemical potential. It is the absence of this term that leads to the vanishing of pairing below a certain finite critical coupling strength. Following steps completely analogous to the ones leading from Eq.(11) to Eq.(13), we obtain the gap equation

$$\frac{\hbar\omega}{\nu G} = \sum_{n=0}^{2n_F} \frac{1}{\sqrt{(n - n_F - 1/2)^2 + (\Delta/\hbar\omega)^2}} \quad (17)$$

with G still defined by Eq.(14) and the scaling factor $\nu = 2^{3/2}/3$ again approximating the n dependence of the radial overlap integrals. The critical coupling strength G_c below which there is no pairing is found by setting $\Delta = 0$ in Eq.(17). Neglecting terms of $\mathcal{O}(n_F^{-1})$, we obtain

$$G_c = \frac{3\hbar\omega}{2^{5/2}\ln(4e^\gamma n_F)}. \quad (18)$$

Using Eq.(18) and expanding Eq.(17) in the small parameter $\Delta/\hbar\omega$, we find

$$\frac{\Delta}{\hbar\omega} = \begin{cases} 0 & , \ G < G_c \\ \left[\frac{3\hbar\omega}{2^{3/2}7\xi(3)}\right]^{1/2}\sqrt{\frac{1}{G_c} - \frac{1}{G}} & , \ G \ge G_c \end{cases} \quad (19)$$

with $\xi(3) = \sum_{n=1}^{\infty} n^{-3} \simeq 1.202$. Equation (19) should be compared to Eq.(15). We see that the main difference is that when there is a harmonic oscillator shell at the chemical potential, the pairing occurs as soon as there is an infinitesimal attraction between the particles. When the chemical potential is between two shells, there is only pairing when the coupling is above a certain critical coupling strength G_c as there is zero density of states at the chemical potential.
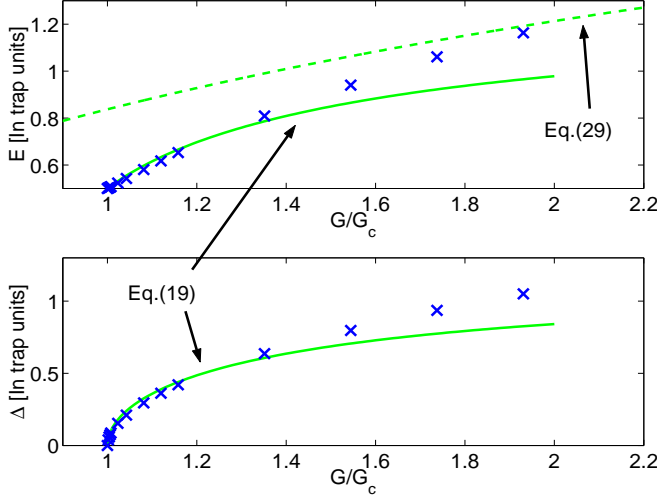
FIG. 4. The lowest l averaged quasi particle energy $E/\hbar\omega$ (a) and the pairing strength $\Delta/\hbar\omega = [E^2 - (\hbar\omega)^2/4]^{1/2}/\hbar\omega$ as a function of G/G_c.

In analogy with fig.(2), we plot in fig.(4) the lowest l averaged quasi particle energy as a function of G/G_c. The line is Eq.(19) and the ×'s are obtained from numerical calculations with $\mu_F = 52\hbar\omega$. As before, we conclude from Eq.(19) that Δ as a function of G/G_c is independent of n_F in the intra-shell pairing regime. Of course, the size of the system is important when determining G_c as is apparent from Eq.(18). Note that the lowest quasi particle energy E is calculated as $E = (\xi_{n_F}^2 + \Delta^2)^{1/2}$ with $\xi_{n_F} = \hbar\omega/2$ and Δ given by Eq.(19). To enable a more direct comparison between the numerical results for the pairing strength and Eq.(19), we also plot $\Delta = (E^2 - \xi_{n_F}^2)^{1/2}$. The observable in an experiment that probes single particle excitations is of course the excitation energy E and not Δ. We see that there is excellent agreement between the numerical results and Eq.(18)-(19) for $\Delta/\hbar\omega \lesssim 1/2$. The approximate analytical formulae predict very well the critical coupling strength and the size of the pairing for small $\Delta/\hbar\omega$ where only intra shell pairing is significant. As in sec.(III A), the pairing between particles in different harmonic oscillator shells become important when $\Delta/\hbar\omega \sim \mathcal{O}(1)$ and the intra shell pairing theory breaks down.

Pairing between just two shells was studied in the context of nuclear structure where similar results were found. Comparing to experimental data [11] only qualitative agreement was found. The nuclear spectra are complicated by stronger anharmonic mean field potentials and the finite range of the nucleon-nucleon interaction as well as spin and spin-orbit dependences. For atomic traps the results presented here should be more accurate as the pseudo potential approximation for the atom-atom interaction is expected to work very well for low atomic densities, and since the mean field is weaker.

C. Effect of the Hartree field

We have sections III A-III B ignored the Hartree field which induces an energy shift $\tilde{\xi}_{nl}$ as given by Eq.(6) of the levels within a given harmonic oscillator shell. In this section, we will examine the effect of this mean field induced spread in the harmonic oscillator shell energies on the pairing. The gap equation including the Hartree field becomes in complete analogy with Eq.(11)

$$\Delta_{nl} = \frac{|g|}{2} \sum_{n',l'} \frac{2l'+1}{4\pi} \frac{\Delta_{n'l'}}{E_{n'l'}} \int_0^\infty dr r^2 \tilde{R}_{nl}^2(r) \tilde{R}_{n'l'}^2(r) \tag{20}$$

with quasi particle energies

$$E_{nl} = \sqrt{\tilde{\xi}_{nl}^2 + \Delta_{nl}^2} \tag{21}$$

and $\tilde{R}_{nl}(r)$ being the solution to the radial Schrödinger equation including the Hartree field. From Eq.(6), we see that the energy spread of a given shell due to the Hartree field is $|\tilde{\xi}_{nl=0,1} - \tilde{\xi}_{nl=n}| \propto n^{3/2}a/a_{osc}$ whereas the size of the pairing assuming completely flat shells is given by Eq.(15) [or Eq.(19)]. Thus, for large n_F the Hartree field splits the different l levels within the same shell sufficiently so that the pairing occurs only within one (or a few) energy levels $\tilde{\xi}_{n_F l}$ close to the chemical potential [9]. Assuming that one level $\tilde{\xi}_{n_F l}$ is at the chemical potential (i.e. $\tilde{\xi}_{n_F l} = 0$), only this level will contribute to the pairing for weak coupling and Eq.(20) becomes

$$\Delta_{n_F l} = \frac{|g|}{2} \frac{2l+1}{4\pi} \int_0^\infty dr r^2 \tilde{R}_{n_F l}^4(r). \tag{22}$$

This equation is straightforward to solve as we simply have to evaluate the radial integral. For instance, for $l = n_F$, we obtain:

$$\frac{\Delta_{n_F l = n_F}}{\hbar\omega} = \frac{|a|/a_{osc}}{\sqrt{\pi}}. \tag{23}$$

Equation (23) agrees with the results derived in ref. [9] using the seniority scheme.

For Eq.(23) to be valid, we need $\Delta_{n_F l} \ll |\tilde{\xi}_{n_F l} - \tilde{\xi}_{n_F l \pm 2}|$. Otherwise, the levels $\tilde{\xi}_{n_F l \pm 2 \pm 4 \ldots}$ away from the chemical potential will contribute significantly to the pairing and the assumption that only particles in the level $\tilde{\xi}_{n_F l} = 0$ form Cooper pairs leading to Eq.(23), will be incorrect. In the discussion following Eq.(15), we concluded that for $\ln(n_F)G \gtrsim 0.1\hbar\omega$ levels away from the chemical potential with normal phase energies $\xi_n = (n - n_F)\hbar\omega$ contributed significantly to the pairing (see Fig. 2). Equation (20) with one level at the chemical potential ($\tilde{\xi}_{n_F l} = 0$) is completely analogous to Eq.(11); ignoring the contribution to the pairing from $n \neq n_F$ shells in Eq.(20) the essential difference between the two equations is the level spacing between the normal phase energies which is $\hbar\omega$ in Eq.(11) and $\tilde{\xi}_{n_F l} - \tilde{\xi}_{n_F l \pm 2}$

in Eq.(20). Thus, a similar analysis on Eq.(20) yields that the contribution from states $\xi_{n_F l'} \neq 0$ to the pairing can be ignored if $|\tilde{\xi}_{n_F l} - \tilde{\xi}_{n_F l \pm 2}| \gg \Delta_{n_F l} \ln(n_F)$ with $\Delta_{n_F l}$ given by Eq.(23). For $l = n_F$ which gives the maximum $|\tilde{\xi}_{n_F l} - \tilde{\xi}_{n_F l \pm 2}|$, this condition yields [using Eq.(6) and Eq.(23)] $n_F \gg 200$. That is, only for rather large systems with $\mu_F \gg 200\hbar\omega$ (corresponding to $N \gg 10^6$ particles trapped), is the pairing for weak coupling only significant in the level $\tilde{\xi}_{n_F l_F} = 0$ at the chemical potential and Eq.(23) is valid. If the chemical potential is at a level with $l < n_F$ (i.e. $\tilde{\xi}_{n_F l} = 0$ with $l < n_F$), the Hartree splitting of the levels is smaller than for $l = n_F$ and the condition for single (n_F, l) pairing becomes even more strict [9].

The assumption in sec.III A-III B that the Hartree field can be neglected such that the harmonic oscillator shells are completely flat, is consistent if $\Delta > |\tilde{\xi}_{n_F l=0,1} - \tilde{\xi}_{n_F l=n_F}|$ with Δ given by Eq.(15) [or Eq.(19)]. From Eq.(6), we have $|\tilde{\xi}_{n_F l=0,1} - \tilde{\xi}_{n_F l=n_F}| \simeq (5/32)n_F G$. Using this and Eq.(15) in the very weak coupling regime with $\Delta = G$, we get the condition $n_F \lesssim 6$ for the validity of neglecting the Hartree field. For stronger coupling where pairing in the shells away from the chemical potential is important, we of course obtain that the neglect of the Hartree field is consistent for larger n_F, since Eq.(15) gives $\Delta > G$. In particular, for $\Delta \sim 0.5\hbar\omega$ which is the approximate maximum value for which the intra shell pairing assumption holds, we obtain that Eq.(15) is valid for systems with $n_F \lesssim 30$.

In order to examine the influence of the Hartree field, we have plotted in fig.(2)(b) as +'s the lowest quasi particle energy (for which $\tilde{\xi}_{nl} = 0$ such that $E_{n_F l} = \sqrt{\Delta_{n_F l}^2 + \tilde{\xi}_{nl}^2} = \Delta_{n_F l}$) including the effect of the Hartree field in order to compare to the results neglecting the Hartree field. We keep the number of particles trapped the same with or without the Hartree field. Since $n_F = 50 > 30$, according to the analysis above the inclusion of the Hartree field should yield a significant modification of the pairing as compared to the analysis presented in sec.III A. As expected, we see that in the intra shell pairing regime the Hartree field suppresses the pairing as it introduces a splitting of the levels in the shell at the chemical potential such that the density of states for $\tilde{\xi}_{nl} = 0$ is reduced. For stronger interaction, where there is pairing between particles in different harmonic oscillator shells, the effect of the Hartree field is to increase the pairing strength. This is because in this regime the Hartree field compresses the gas increasing the density $\rho(r = 0)$ thereby increasing the effective interaction strength $k_F(r = 0)|a|$ [See Eq.(4)]. We see that Eq.(15) gives a qualitatively correct description of the pairing strength for this set of parameters since $n_F = 50$ is an intermediate value where the pairing in the intra shell regime is not in the limit where the Hartree field can be ignored, but also far away from the limit where there is only pairing within the level $\tilde{\xi}_{nl} = 0$.

IV. PAIRING IN THE $\Delta(R = 0) \gg \hbar\omega$ LIMIT

In this section, we will derive an analytical expression for the lowest single particle energy in the regime, where the pairing field $\Delta(r)$ is much larger than $\hbar\omega$, yet still in the dilute limit so that $\Delta(r) \lesssim E_F$. We will show that the strong pairing between particles in different shells leads to a break-down of intra shell pairing ansatz of secs.III A-III B; we are in the *inter* shell pairing regime.

When $\Delta(r = 0) \gg \hbar\omega$ the local or TF coherence length in the center of the trap [10]

$$\xi(r = 0) = \frac{k_F(r = 0)}{\pi m \Delta(r = 0)} \tag{24}$$

is smaller than the size of the system. The coherence length in general determines the length scale over which the pairing field can vary. In this regime, the shell structure of the trap levels can be ignored and the gas behaves in many ways as a quasi-homogeneous bulk system. In nuclei gaps are always smaller than $\hbar\omega$ by an order of magnitude [11]. Thus trapped atoms provide a bridge between condensed matter and nuclear physics for studying superfluid properties.

The pairing field $\Delta(r)$ in Eq.(7) in general increases with $r \to 0$ in the bulk regime. When $\Delta(r = 0) \gg \hbar\omega$, we have $\xi_{BCS}(r = 0)/R_{TF} \ll 1$. One can in this regime use a semiclassical theory developed in Ref. [12] to obtain an analytical expression for the lowest quasi particle energy. As discussed in Ref. [12], the lowest excitations are concentrated in the region around the minimum of $\Delta(r) + U_0(r) - \mu_F$. The lowest excitations have energies $E_{\eta l}$ significantly lower than $\Delta(r = 0)$ and can be denoted "in gap excitations". Their wave-functions are suppressed in the regions where $E_{\eta l} < \Delta(r)$ and $E_{\eta l} + \mu_F < U_0(r)$. To illustrate this, we plot in Fig. (5) the four Bogoliubov wave functions $[u_{\eta l}(r), v_{\eta l}(r)]$ with lowest energy $E_{\eta l}$ for $l = 0$, $\mu_F = 51.5\hbar\omega$ and $G \simeq 0.34\hbar\omega$.
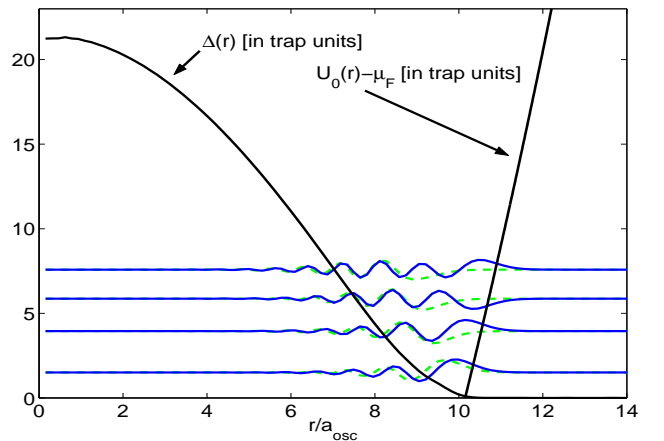
FIG. 5. The lowest 4 Bogoliubov wavefunctions $u_{\eta l}(r)$ and $v_{\eta l}(r)$ in units of a_{osc}^{-3} for $l = 0$, $\Delta(r)$, and $U_0(r) - \mu_F$ in units of $\hbar\omega$.

The solid lines are the $u_{\eta l=0}(r)$ and the dashed lines are the $v_{\eta l=0}(r)$. The wave functions are centered horizontally along a y-value equalling their excitation energy in units of $\hbar\omega$. We also plot $\Delta(r)$ and $U_0(r) - \mu_F$ to illustrate how the lowest quasi particle excitations with energies $E_\eta \ll \Delta(r = 0)$ are centered at the edge of the cloud where $\Delta(r) + U_0(r) - \mu_F$ has a minimum.

For $E_\eta \ll \Delta(r = 0)$, a semiclassical analysis yields the following quantization condition for the $l = 0$ states [12]:

$$(\eta + \frac{1}{2})\frac{\pi}{2}\hbar\omega = \int_{r_c}^{R_{TF}} dr \frac{\sqrt{E_\eta^2 - \Delta(r)^2}}{\sqrt{R_{TF}^2 - r^2}} \qquad (25)$$

with $\eta = 0, 1, \ldots$. Here, r_c is the left turning point determined by $\Delta(r_c) = E_\eta$. For $\Delta(r = 0) \gg \hbar\omega$ we have $1 - r_c/R_{TF} \ll 1$. The centrifugal barrier, present for $l > 0$ plays a minor role since the Bogoliubov wavefunctions are suppressed by $\Delta(r)$ in the region where the centrifugal potential is significant. Therefore the l-dependence of E_η is weak and only when l becomes comparable to n_F does the centrifugal potential affect the lowest energy states for a given l by increasing its energy.

In a uniform system the pairing gap is

$$\Delta \simeq \kappa \frac{p_F^2}{2m} e^{-\pi/2k_F|a|} . \qquad (26)$$

The prefactor $\kappa = 8e^{-2}$ within the usual BCS theory but is further reduced by a factor $(4e)^{-1/3}$, when induced interactions are included [13].

In a non-uniform system such as the h.o. traps we can use the local density (or TF) approximation in the $\Delta(r = 0) \gg \hbar\omega$ regime, where the discrete level structure is of minor importance as compared to the strong pairing field. A Thomas-Fermi treatment yields

$$\Delta(r) \simeq \kappa\mu_F(1 - r^2/R_{TF}^2)e^{-\pi/2k_F(r)|a|} . \qquad (27)$$

The gap decreases rapidly near the surface and we can therefore neglect the gap in the region $r_c < r < R_{TF}$ [see Fig. (5)]. The semiclassical quantization condition thus simply gives

$$E_\eta = \frac{\pi}{2} \frac{(\eta + \frac{1}{2})\hbar\omega}{\arccos(r_c/R_{TF})} \qquad (28)$$

Here, the turning point given from $E_\eta = \Delta(r_c)$ is now determined from the gap of Eq.(27). We thus obtain in the $\Delta(r = 0) \gg \hbar\omega$ regime

$$G \simeq \frac{32E_\eta}{15\pi^2(\eta + 1/2)} \left\{ \ln \left[\frac{\kappa(\eta + 1/2)^2\pi^2}{4} \frac{n_F(\hbar\omega)^3}{E_\eta^3} \right] \right\}^{-1} , \qquad (29)$$

from which the quasi particle particle energy E_η can be found by inversion from the coupling strength G defined in Eq.(14).

The lowest quasi particle energy, E_0, from Eq. (29) (plotted as a dashed line) is compared with the numerical results in fig.(2) and fig.(4). We see that the agreement between the semi classical prediction and the numerical results is good for $E \gtrsim \hbar\omega$ where $\Delta(r = 0) \gg \hbar\omega$. Note that in the inter shell pairing regime, the position of the chemical potential with respect to the Harmonic oscillator levels is unimportant as the lowest quasi particle energy is determined by the geometry of the minimum of $\Delta(r) + U_0(r)$. Thus, Eq.(29) agrees well with the numerical results for the parameters relevant for both fig.(2) (partly filled shell) and fig.(4) (filled shell). Combined with the theory presented in sec.(III), we therefore have a theory describing the strength of the pairing fairly well in the regimes $\Delta \lesssim \hbar\omega/2$ and $\Delta(r = 0) \gg \hbar\omega$. In the weak coupling regime, the pairing is between particles within the same shell whereas for stronger interaction, there is pairing between particles in different shells and the lowest energy excitations are states localized in the surface region around the minimum of $\Delta(r) + U_0(r)$.

Equation (29) for the lowest quasi particle energy should be compared with Eq.(27) giving the size of the pairing field in the center of the trap. We see that contrary to the homogeneous case, the lowest pairing energy in general is different from the size of the pairing field even in the quasi homogeneous bulk limit; it grows much slower with G than $\Delta(r = 0)$.

V. CONCLUSION

In this paper, we considered the properties of the elementary excitations of a superfluid trapped atomic Fermi gas. The nature of the paired state was shown to undergo transitions between several different regimes as the number of particles (or the h.o. quantum number $n_F = (3N)^{1/3}$) and the strength of the interaction are varied. Three regions emerge:

- For weak coupling, $G \ln(n_F) \lesssim 0.1$, the Cooper pairs were shown to be formed between states in the h.o. shell at the Fermi surface only. In this limit, it was demonstrated that both the position of the chemical potential with respect to the harmonic oscillator shells and the size of the Hartree field, are strongly influencing the nature of the paired stated. The pairing gap is $\Delta = G$ for sufficiently few particles in the trap, $n_F \lesssim 10$, but for more particles the mean field splits the single particle levels and reduce the pairing. For $n_F \gg 100$ the pairing is reduced to that in a single l-level.

- For interactions such that $0.1 \lesssim G \ln(n_F)/\hbar\omega \lesssim 1/2$ Cooper pairs are still essentially only formed between states within the same shell. However, there is pairing in many shells besides that at the Fermi level yielding a gap significantly larger than $\Delta = G$.

- For strong interactions, $G \ln(n_F)/\hbar\omega \gtrsim 1/2$, the pairing field exceeds $\Delta(r = 0) \gtrsim \hbar\omega$. The coherence length is shorter than the system size, and

the gas can for many purposes be regarded as a quasi-homogeneous bulk system The Cooper pairs are formed between particles in different shells and the elementary excitations are confined spatially to the surface of the gas.

It should be noted that the transitions between the regions described above are smooth contrary to thermodynamic phase transitions. The analytical formulae appropriate for the various regimes were compared with numerical calculations showing excellent agreement. The results presented in this paper suggest, that by varying the number of particles and/or their interaction strength the trapped atomic gases can behave either essentially as giant nuclei (Sec.III) or as bulk systems (Sec.IV). They thus provide an intriguing link between uniform systems explored in condensed matter physics and finite systems relevant for nuclear physics, quantum dots, etc.

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